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THE EVALUATION OF QUANTUM INTEGRALS

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Rather a long time after its publication, my attention was drawn to a paper by Mr. E. C. Kemble¹ dealing with the evaluation of the integral

$$J = 2 \int_a^b \sqrt{f(q)} dq, \quad (1)$$

where a and b denote the roots of the radicand. Before preparing his own method of computation, Mr. Kemble criticizes two procedures used by other authors and rejects them as inadequate and even as erroneous. This judgment cannot remain uncontradicted for in reality these procedures are both perfectly correct and very efficient. Since the integral under consideration was first introduced into the theory of quanta by the writer of this note² in order to formulate his quantum conditions for conditionally periodic motions, the moral obligation of putting things right is his.

The first method to which Mr. Kemble objects is used when $f(q)$ can be expressed in the form

$$f(q) = \varphi(q) + \alpha\psi(q) \quad (2)$$

where $\varphi(q)$ is quadratic in q , α denotes a constant and $\alpha\psi(q)$ is small compared with $\varphi(q)$. The most obvious method consists in developing $\sqrt{f(q)} = Q(\alpha)$ in powers of α

$$Q(\alpha) = Q(o) + \alpha Q'(o) + \frac{\alpha^2}{1.2} Q''(o) + \dots \quad (3)$$

and integrating this series termwise. Mr. Kemble remarks that the integrals of the higher terms cannot be calculated, "because the higher derivatives of $\sqrt{f(q)}$ with respect to α become infinite at $q=a$ and $q=b$." It seems to me that the latter statement is not sufficient to draw such a conclusion; in the coefficients of series (3) there is, indeed, substituted o for α , so that they remain finite at the values $q=a$ and $q=b$, and so that the case requires a further investigation. That the roots of the function $\varphi(q)$ can also in a certain sense be regarded as limits of integration can be deduced only if the method of complex integration is used, but the latter supplies at the same time the means for overcoming the difficulty of the integrand becoming infinite at those points. This method was given by Riemann³ just for the treatment of integrals of the type (1) and was first applied by Sommerfeld⁴ to problems of the theory of quanta. It is not necessary to expand upon it for it is explained with much detail in the

books both of Riemann and of Sommerfeld.⁵ Therefore the assertion of Mr. Kemble that the expansion (3) is applicable only when terms of the second and higher order in α are negligible is entirely unfounded. An expansion of this type was first introduced into the theory of quanta by the present writer in his work on the Stark effect and, as a matter of fact, the computation was carried through by him not only for the term of the first order, but also for the term of the second order⁶ and proved to be as easy as can be desired.

The method followed by F. Tank in a paper referred to by Mr. Kemble is but a slight modification of this procedure. The purpose of Tank is to find an expansion for the integrand $\sqrt{f(q)}$ when it is not given in the form (2). This purpose is reached by developing $f(q)$ in a power series from the point $q=d$, which makes $f(q)$ a maximum. If $q-d=\xi$ and if H denotes the maximum value of $f(q)$, this function can be represented in the form

$$f(q) = H - \alpha\xi^2 - (\beta\xi^3 + \gamma\xi^4 + \dots) = H - \alpha\xi^2 - \Delta,$$

wherefrom

$$\sqrt{f(q)} = \sqrt{H - \alpha\xi^2} - \frac{1}{2} \frac{\Delta}{\sqrt{H - \alpha\xi^2}} - \frac{1}{8} \frac{\Delta^2}{(\sqrt{H - \alpha\xi^2})^3} - \dots$$

To this series the method of complex integration can be applied termwise in exactly the same way as to expansion (3). Since the complex path of integration amounts to a real one between the roots of the radicand $H - \alpha\xi^2$, whenever this real integral is convergent. Tank was perfectly justified in taking as limits $-(H/\alpha)^{1/2}$ and $+(H/\alpha)^{1/2}$. Moreover I cannot agree with the opinion of Mr. Kemble that "the expansion is not usually convergent throughout the interval of integration." It can be shown in a general way that the problem of convergence cannot lead to any difficulties.

Summarizing, we can say that both methods in question are correct and have been successfully applied to the treatment of important problems. The new procedure proposed by Mr. Kemble may answer its purpose as a method of computation, but it surely does not equal the old ones in directness and mathematical elegance.

¹ E. C. Kemble, *Proc. Nat. Acad. Sci.*, **7**, 1921 (283).

² Paul S. Epstein, *Ann. Physik.*, **50**, 1916 (489).

³ B. Riemann, *Schwere, Elektrizität, Magnetismus*, section 27, Hannover, 1880.

⁴ A. Sommerfeld, *Physik. Zs.*, **17**, 1916 (500).

⁵ A. Sommerfeld, *Atombau u. Spektrallinien*, pp. 476-482. Braunschweig, 1921.

⁶ P. S. Epstein, *Ann. Physik.*, **51**, 1916 (184).